Original Article

Zagreb Index Of Signed Labeled Graphs UsingDomination Degree And Of The Drug Cis-Diamminedichloroplatinum(II)

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Abstract

In this paper, we establish the first and second Zagreb indices for labelled signed graphs utilizing the ideas of dominance degree and minimum dominating sets. We discover several generalizations for these indices for a number of common labeled signed graphs and explain the outcomes. We also calculate Zagreb Indices for the drug cis-diamminedichloroplatinum(II)(cisplatin).

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1. INTRODUCTION

The Molecular descriptors[4], which are graph invariants, give us details on the chemicalmolecule's internal structure. One of the topological indexes is the Zagreb index.

Definition 1.1 *[1, 3]The first Zagreb index, which is represented by the notation $M_1(G)$, hasthe following definition:*

$$M_1(G) = \sum_{i=1}^{n} d_i^2$$

[1, 3]The second Zagreb index, which is represented by the notation $M_2(G)$, has the following definition:

$$M_2(G) = \sum d_i d_j \quad \text{, where i,j= 1 to n.}$$

Definition 1.2 *[5]A signed graph $\Sigma = (G, \sigma) = (W, E, \sigma)$ is a graph which assigns a sign $+$ or $-$ to every vertex in G.*

Definition 1.3 *[8]A dominant set in the context of a graph G is a subset D of its vertices, andthis means that every vertex in G either belongs to D or has a neighbour who does.*

Definition 1.4 *[8]A dominating set in a graph is said to be minimal if it does not constitutea suitable subset of any other dominating set in the graph.*

Please go to for further information on dominance in graphs [6].

Definition 1.6 *[7]The absolute value of the difference between a vertex's positive and negativedegrees is called its signed degree (ssdeg).*

$$sdeg(v) = |deg^{+}[\sigma(v)] - deg^{-}[\sigma(v)]|.$$

2. Zagreb Index for signed labeled graph using domina-tion degree

Hanan A, Anwar A, and Rubi S Morgan developed the minimum dominating set and domi-nance degree in [8] and provided the dominance degree for a number of common graphs. Weuse domination degree for a few common graphs to define the Zagreb indices of labelled signedgraphs and discover generalizations for the indices. Let G be a straightforward graph. The pro-cedures below are used to obtain the labelled signed graph of G using the dominance degree. Step one is to write the domination degree of the specific graph on the vertex.
Step two is to give a positive sign to the vertex that has an even degree label.Step three is to give the vertex with the odd degree label a negative sign.
Step four is to ascribe to the edges the signs that result from multiplying the appropriate ver-tices together.
Calculate each vertex's signed degree in the graph G in step five. We use dominance degree todefine the topological index for labelled signed graphs.

Definition 2.1 *Let's call this the labeled signed graph with a non-empty vertex set, or LS_Gfor short. The first Zagreb index for the variable* $_G$ *is given by the symbol* $FZ(_G)$*), andits definition is as follows:*

$$FZ(LS_G) = \Sigma \quad d_d(w_i) \; (sdeg(w_i))^2.$$

where limits of summation is i= 1 to n.

Definition 2.2 *The second Zagreb index for* LS_G *is denoted by* $SZ(LS_G)$ *and is defined as*

$$SZ(LS_G) = \Sigma \quad d_d(w_i) \; (sdeg(w_i)) \; d_d(v_j) \; (sdeg(v_j)).$$

where limits of summation is i,j = 1 to n.

2.1 Complete Labeled Signed Graph.

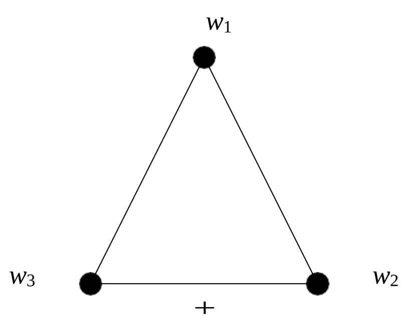


Figure 1: Complete Graph(K_n)

The dominance degree for the entire graph's vertices, as shown in figure 1 below, is one. Given that there are an uneven number of vertices, we label them with a negative sign. Weassign the product of the corresponding vertices to the edges as a label. FZ(K_n)=12 and also we calculate second Zagreb as follows,

$$SZ(K_n) = \Sigma^{n}_{+} \quad d_d(u_i) \; (sdeg(u_i)) \; d_d(u_j) \; (sdeg(u_j))$$

$$= (1 \times 2 \times 1 \times 2) + (1 \times 2 \times 1 \times 2) + (1 \times 2 \times 1 \times 2)$$
$$= 4 + 4 + 4$$
$$= 12$$

Theorem 2.1 *The first Zagreb index is given as* $FZ(K_{1,n-1}) = 2\ ^{n}C_2$*, if* $LS(K_{1,n-1})$ *is the labelled signed star graph.*

Proof. Consider the labelled signed star graph $LS(K1, n-1)$. We assign the number one to each vertex of the star network since each vertex's domination degree equals one. Give each vertex a negative sign. The product of the corresponding vertices should be written on the edges. Consequently, the sdeg of vertex u_1 is 1 while the sdeg of the remaining vertices is$(n-1)$. Now,

$$FZ(K_{1,n-1}) = \sum_{i=1}^{n} d_d(u_i)\ (sdeg(u_i))^2$$

$$= d_d(u_1)\ [sdeg(u_1)]^2 + \sum^n d_d(u_i)\ [sdeg(u_i)]^2$$
$$= 1\ (n-1)^2 + (n-1)(1)(1)^2$$
$$= 2\ {}^nC_2$$

Theorem 2.2 *If $LS(Kn)$ is the labelled signed complete graph, then $FZ(K_n) = 2\ (n\ \text{-}1)\ {}^nC_2$ is the first Zagreb index.*

Proof. Consider a labelled signed complete graph, $LS(Kn)$. Since all of the vertices of the fullgraph have domination degrees of 1, we assign the number 1 to each vertex. Give each vertexa negative sign. The product of the corresponding vertices should be written on the edges.

Consequently, each of these vertices has a signed degree of $(n-1)$. Now,

$$FZ(K_n) =\sum^n d_d(u_i)\ (sdeg(u_i))^2$$
$$= (n)\ 1\ (n-1)^2$$
$$= 2\ (n-1)\ {}^nC_2$$

Theorem 2.3 *The first Zagreb index is given as $FZ(DSr, n) = 4\ [(n+1)^2+n]$, if $LS(DSr, n)$ is the labelled signed double-star graph.*

Proof. Consider a labelled signed double-star graph, $LS(DS_{r,n})$. We assign the number two to each vertex of the star network since the ddeg is two for all of its vertices. Give each vertexa positive sign. The product of the corresponding vertices should be written on the edges.

∴ The signed degree of vertex u_1 is $(n+1)$, and the remaining vertex's signed degree is 1. Now,

$$FZ(DS_{r,n}) = \sum^n d_d(u_i)(sdeg(u_i))^2$$

$$= d_d(u_1)\ [sdeg(u_1)]^2 + \sum^n d_d(u_i)\ [sdeg(u_i)]^2$$
$$= 2\ (n+1)^2\ 2 + (2n)(1)(1)^2$$
$$= 4\ [(n+1)^2 + n]$$

Theorem 2.4 *If $LS(Wdr^n)$ is the labelled signed windmill graph, then $FZ(Wdr^n) = 4n^2$ is the first Zagreb index.*

Proof. Consider a labelled signed windmill graph, $LS(Wdr^n)$. We label the centre vertex with one and all the other vertices of the windmill network with $(r\text{-}1)^{(n-1)}$ since the ddeg for the windmill graph is 1 for the centre vertex and $(r\text{-}1)^{(n-1)}$ for the rest vertices. Give thecore vertices a negative sign while giving the other vertices a positive sign. The product of the corresponding vertices should be written on the edges. Therefore,u_1's signed degree is $(2n)$ and the signed degrees of the remaining vertices are both 0. Now,

$$FZ(Wdr^n) = \sum^n d_d(u_i)\ (sdeg(u_i))^2$$

$$= 1\ (2n)^2 + (n-1)(1)(0)^2$$
$$= 4n^2$$

Proof. Let $LS(Bn)$ be a graph of a labelled signed book. Label the central vertices of the book graph with three and all other vertices with $2n\text{-}1 + 1$ because the centre vertices of the book graph have a dominance degree of three and the rest vertices have a ddeg of $2n\text{-}1 + 1$. Give the opposite sign to all the other vertices and a negative sign to the. The product of the corresponding vertices should be written on the edges. As a result, u_1's signed degree is $(\Gamma + n)$ and

the sdeg of the rest vertices are both 2.
Now,

$$FZ(B_n) = \Sigma_{i=1}^{n} d_d(u_i)\ (sdeg(u_i))^2$$
$$= 3\ (n+1)^2\ (2^{n-1}+1)(2)^2\ 2n$$
$$= 6(n+1)^2\ + 8n\ (2^{n-1}+1)$$

Theorem 2.6 *If n is odd and $LS(K_{m,n})$ is the labelled signed complete bipartite graph, then $FZ(K_{m,n}) = (n^3)\ (n+1)$ is the first Zagreb index.*

Proof. Consider the labelled signed complete bipartite graph $LS(K_{m,n})$, where n is not even. All of the vertices of the whole bipartite graph are labelled in accordance with the fact that the ddeg for the entire graph is $d(v_i)$ +1. Give each vertex a positive sign. The product of the corresponding vertices should be written on the edges. Therefore, all of these vertices have a signed degree of n. Labeled signed complete bipartite graph's initial Zagreb index is

$$FZ(K_{m,n}) = \Sigma_{i=1}^{n} d_d(u_i)\ (sdeg(u_i))^2$$
$$= n\ (n+1)\ n^2$$
$$= (n^3)\ (n+1)$$

Theorem 2.7 *If n is even and $LS(K_{m,n})$ is the labelled signed complete bipartite graph, then $FZ(K_{m,n}) = (n^3)\ (n+1)$ is the first Zagreb index.*

Proof. Let $LS(K_{m,n})$ be an even-numbered labelled signed complete bipartite graph. Allof the vertices of the whole bipartite graph are labelled in accordance with the fact that the ddeg for the entire graph is $d(v_i)$ +1 . Give each vertex a negative sign. The product of the corresponding vertices should be written on the edges. Therefore, all of these vertices have a signed degree of n. Labeled signed complete bipartite graph's initial Zagreb index is

$$FZ(K_{m,n}) = \Sigma_{i=1}^{n} d_d(u_i)\ (sdeg(u_i))^2$$
$$= n\ (n+1)\ n^2$$
$$= (n^3)\ (n+1)$$

Theorem 2.8 *The second Zagreb index is given as, $\frac{2(n-1)}{n}\ {}^{n}C_2$,* if $LS(K_{1,n-1})$ is the labelled signed star graph.

Proof. Consider the labelled signed star graph $LS(K_{1,n-1})$. We assign the number oneto each vertex of the star network since each vertex's domination degree equals one. Give each vertex a negative sign. The product of the corresponding vertices should be written on the edges. Consequently, the signed degree of vertex u_1 is 1 while the sdeg of the remaining vertices is $(n-1)$. The labelled signed star graph's second Zagreb index is

$$SZ(K_{1,n-1}) = \Sigma_{i=1}^{n} d_d(u_i)\ (sdeg(u_i))\ d_d(u_j)\ (sdeg(u_j))$$
$$= \frac{2(n-1)}{n}\ {}^{n}C_2$$

Theorem 2.9 *The second Zagreb index is given as $SZ(K_n) = 2\ (n-1)\ {}^{n}C_2$, , if $LS(K_n)$ is thelabelled signed complete graph.*

Proof. Consider a labelled signed complete graph, $LS(K_n)$. Since all of the vertices of the fullgraph have domination degrees of 1, we assign the number 1 to each vertex. Give each vertexa negative sign. Put the product of the corresponding vertices on the edges. As a result, allof these vertices have a signed degree of (n-1). Labeled signed complete graph's second Zagreb index is

$$SZ(K_n) = \Sigma_{i=1}^{n} d_d(u_i)\ (sdeg(u_i))\ d_d(u_j)\ (sdeg(u_j))$$

$= (n)\ 1\ (n-1)^2$
$= 2\ (n-1)\ {}^nC_2$

Theorem 2.10 *The second Zagreb index is given as* $SZ(DSr, n) = 12(n)^2 - 8n$, *if* $LS(DS_{r,n})$ *is the labelled signed double-star graph.*

Proof. Consider a labelled signed double-star graph, $LS(DSr, n)$. We assign the number twoto each vertex of the star network since the ddeg is two for all of its vertices. Give each vertexa positive sign. The product of the corresponding vertices should be written on the edges.

Therfore, the signed degree of vertex u_1 is $(n + 1)$, and the remaining vertex's signed degree is one.

The labelled signed star graph's second Zagreb index is

$$SZ(DS_{r,n}) = \Sigma^n_{i=1} d_d(u_i)\ (sdeg(u_i))\ d_d(u_j)\ (sdeg(u_j))$$

$$= 2\ (n)\ 2\ (1)\ (2n-2) + 2\ (n)\ (2)\ (n)$$
$$= 12(n)^2 - 8n$$

Theorem 2.11 *Second Zagreb index for labelled signed book graph* $LS(Bn)$ *is given by* $SZ(B_n) = 4(2^{n-1} + 1)\ [3\ (n + 1)^2 + n\ (2^{n-1} + 1)]$ *for any n.*

Proof. Let $LS(B_n)$ be a graph of a labelled signed book. Denote the central vertices of thebook graph with three and all other vertices with $2^{n-1} + 1$ because the centre vertices of thebook graph have a dominance degree of three and the rest vertices have a domination degreeof $2^{n-1} + 1$. Give the opposite sign to all the other vertices and a negative sign to the. The product of the corresponding vertices should be written on the edges. As a result, u_1's signed degree is $(1 + n)$ and the signed degrees of the rest vertices are both 2.

The graph of labelled signed books from Zagreb's second index is

$$SZ(B_n) = \Sigma^n_{i=1} d_d(u_i)\ (sdeg(u_i))\ d_d(u_j)\ (sdeg(u_j))$$

$$= 3\ (n + 1)\ (2^{(n-1)} + 1)\ (2)\ (n + 1)\ (2) + (2^{n-1} + 1)\ (2)\ (2^{n-1} + 1)\ (2)\ (n)$$
$$= 4(2^{n-1} + 1)\ [3\ (n + 1)^2 + n\ (2^{n-1} + 1)]$$

Theorem 2.12 *The second Zagreb index is given as* $SZ(K_{m,n}) = (n^3)\ (n + 1)^2$, *if* $LS(K_{m,n})$ *is the labelled signed complete bipartite graph and n is odd.*

Proof. With n being odd, now $LS(Km, n)$ be a labelled signed complete bipartite graph.

All of the vertices of the whole bipartite graph are labelled in accordance with the fact thatthe ddeg for the entire graph is $d(vi)+1$. Give each vertex a positive sign. The product ofthe corresponding vertices should be written on the edges. Therefore, all of these vertices havea signed degree of n. Labeled signed complete bipartite graph's second Zagreb index is

$$SZ(K_{m,n}) = \Sigma^n_{i=1} d_d(u_i)\ (sdeg(u_i))\ d_d(u_j)\ (sdeg(u_j))$$

$$= n\ (n+1)\ n\ (n+1)\ n$$
$$= (n^3)\ (n+1)^2$$

Theorem 2.13 *If $LS(Km, n)$ is the labeled signed complete bipartite graph and n is even, then the second Zagreb index is provided by $SZ(K_{m,n}) = (n^3)\ (n+1)^2$.*

Proof. Let $LS(Km, n)$ be an even-numbered labelled signed complete bipartite graph. Allof the vertices of the whole bipartite graph are labelled in accordance with the fact that the ddeg for the entire graph is $d(v_i) + 1$. Give each vertex a positive sign. The product of the corresponding vertices should be written on the edges. Therefore, all of these vertices have a signed degree of n. Labeled signed complete bipartite graph's second Zagreb index is

$$SZ(K_{m,n}) = \Sigma^n_{i=1} d_d(u_i)\ (sdeg(u_i))\ d_d(u_j)\ (sdeg(u_j))$$

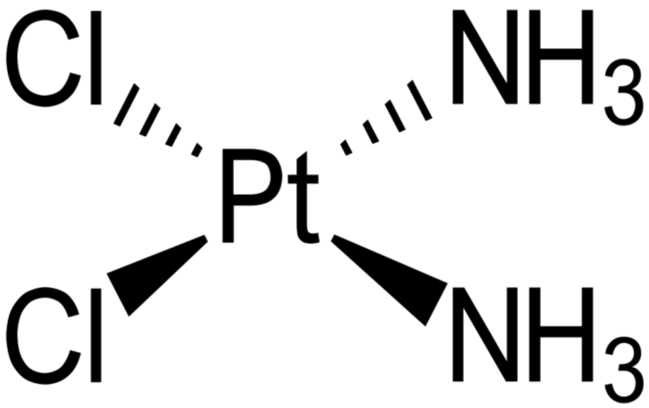
$$= (n^3)\ (n+1)^2$$

Since the signed degree of every vertex in the windmill graph except for the centre vertex is 0,the second Zagreb index value is also 0.

3. Zagreb Index of The Drug Cisplatin

Cancer is a condition that occurs when aberrant cells in one area of the body divide withoutcontrol, which can lead to the development of cancer. These days, there are a great variety of for us to choose from bladder cancer like, cancerous like. Cancers of the lung, brain, breast, cervix,ovary, and other organs, including but not limited to lung cancer, brain cancer, melanoma, breast cancer, and non-Hodgkin lymphoma. Cisplatin[**9**]is a medication that has proven to be quite effective in the fight against cancer. In this study, we calculate the Zagreb index of cisplatin, which is very valuable for future research and development in the treatment of cancersince Zagreb indices are used in analysing the drug structure. This index measures how effective cisplatin is at killing cancer cells.

Structural Formula: $[Pt(NH_3)_2Cl_2]$



Theorem 3.1 *For vertex labeled signed graph of cisplatin $W_L(\Sigma(G))$ where n is odd[10], we have,*

(i) $M_1^-[W_L(\Sigma(G))] = M_1(G)$

(ii) $M_2^-[W_L(\Sigma(G))] = M_2(G)$.

The First and Second Zagreb indices are equal to the First and Second Zagreb indices of Signed Labeled graph of the drug cisplatin. This information may be helpful in finding the behavior or side effects of the drug cis-diamminedichloroplatinum(II).

4. APPLICATION

Machine learning automates developing analytical models from data. AI predicated on the premise that systems can learn from data, detect patterns, and make decisions without human help.

Machine learning is like computational statistics, which predicts with computers. Machine learning algorithms generate a mathematical model using "training data". This model auto- matically makes predictions or judgments. Using data analytics, artificial intelligence, the trainand test data split method, and machine learning, we can create different mathematical modelsto analyze the different physical, chemical, and biological properties of different chemical graphs and drugs by generalizing the topological indices for the same graphs.

5. CONCLUSION

The degree of dominance is used to define labeled signed graphs on the molecular descriptorsfirst Zagreb index and second Zagreb index, and different types of standard signed graphs are shown to show what they look like. The results of generalizing this topological index to all standard graphs are discussed. We have foundout the Zagreb indices for the drug cisplatin and explained the applications of it . We wish to apply machine learning models to identify new topological indices for standard and chemical graphs.

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